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Superfluid-Mott Insulator Transition of Spin-1 Bosons in an Optical Lattice

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Abstract

We have studied superfluid-Mott insulating transition of spin-1 bosons interacting antiferromagnetically in an optical lattice. We have obtained the zero-temperature phase diagram by a mean-field approximation and have found that the superfluid phase is to be a polar state as a usual trapped spin-1 Bose gas. More interestingly, we have found that the Mott-insulating phase is strongly stabilized only when the number of atoms per site is even.

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Superfluid-Insulator (S-I) transition has attracted attention, and has been extensively studied in the context of ^{4}He absorbed in the porous media [1, 2], granular superconductors [3] and Josephson-junction arrays [4]. Recently, Greiner *et al.* [5] has observed an S-I transition of ^{87}Rb atoms trapped in a three-dimensional optical lattice potential by changing the potential depth when the number of atoms par site is an integer. This method is the most ideal way to study the S-I transition. There are no lattice imperfections, and we can easily change the potential depth in order to study both superfluid and insulator phases in a single system.

On the other hand, recent advances of experimental techniques in an optical trap [6, 7] have achieved condensation of spinor bosons. Recent theoretical studies predict a variety of novel phenomena of spinor condensates such as fragmented condensation [8], skyrmion excitations [9, 10, 11, 12] and propagation of spin waves [12, 13].

Here, a natural question is what is expected if the spinor bosons are trapped in an optical lattice. In fact, several unique properties of spinor Bose atoms in an optical lattice have been suggested by Demler and Zhou [14]. They have proposed some possible phases including the superfluid and insulating phases [14], however, no microscopic calculation has been given for their boundaries nor stabilities. In this Letter, we study the S-I transition of spin-1 bosons with antiferromagnetic interaction in an optical lattice at zero temperature when the number of atoms per site is an integer. Using a mean-field approximation [15, 16], we show the zero-temperature phase diagram where the superfluid phase is a polar state as in the case of spinor bosons trapped in a usual harmonic trap. More interestingly, we have found that the Mott-insulating phase is strongly stabilized only when the number of atoms per site is even.

Bosons with hyperfine spin $F = 1$, which include alkali atoms with nuclear spin $I = 3/2$ such as ^{23}Na, ^{39}K and ^{87}Rb, are represented by the Bose-Hubbard model[17] in an optical lattice as

$$\begin{aligned} H = \quad & -t \sum_{<i,j>,\alpha} (a^\dagger_{i\alpha} a_{j\alpha} + a^\dagger_{j\alpha} a_{i\alpha}) - \mu \sum_{i,\alpha} a^\dagger_{i\alpha} a_{i\alpha} \\ & + \frac{1}{2} U_0 \sum_{i,\alpha,\beta} a^\dagger_{i,\alpha,\beta} a^\dagger_{i\beta} a_{i\beta} a_{i\alpha} + \frac{1}{2} U_2 \sum_{i,\alpha,\beta,\gamma} a^\dagger_{i\alpha} a^\dagger_{i\gamma} \mathbf{F}_{\alpha\beta} \cdot \mathbf{F}_{\gamma\delta} a_{i\delta} a_{i\beta}, \end{aligned} \tag{1}$$

where $a_{i\alpha}$ is the annihilation operator for an atom with hyperfine spin α $(= 0, \pm 1)$ at site i

and μ is the chemical potential. $t = -\int d\mathbf{r} w_i^*(\mathbf{r}) \left(-\hbar^2\nabla^2/2M + V_0(\mathbf{r})\right) w_j(\mathbf{r})$ is the hopping matrix element between adjacent sites i and j, where $w_i(\mathbf{r})$ is a Wannier function localized on the ith lattice site, M is the atomic mass and $V_0(\mathbf{r})$ is an periodic potential which characterizes an optical lattice. U_0 (U_2) is the on-site spin-independent (spin-dependent) inter-atom interaction. U_F ($F = 0, 2$) is defined by $U_F = c_F \int d\mathbf{r}|w_i(\mathbf{r})|^4$, where $c_0 = (g_0 + 2g_2)/3$, $c_2 = (g_2 - g_0)/3$, $g_F = 4\pi\hbar^2 a_F/M$, and a_F is an s-wave scattering length for two colliding atoms with total spin F. We assume an antiferromagnetic interaction $U_2 > 0$ ($a_2 > a_0$). This is the case for ^{23}Na atoms.

In a Mott insulating phase with large inter-atom interaction (U_0,$U_2 \gg t$), we obtain an effective Hamiltonian within the second-order perturbation for the hopping parameter t as $H_{eff} = -J_1 \sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j - J_2 \sum_{<i,j>} \left(\mathbf{S}_i \cdot \mathbf{S}_j\right)^2 = -\frac{J_2}{4} \sum_{<i,j>} [(\mathbf{S}_i + \mathbf{S}_j)^2 - 4][(\mathbf{S}_i + \mathbf{S}_j)^2 - 4 + 2/\alpha]$, where $J_1 = 2t^2/(U_0 + U_2)$, $J_2 = \frac{2t^2}{3}\left(\frac{1}{U_0+U_2} + \frac{2}{U_0-2U_2}\right)$, and $\alpha \equiv J_2/J_1 = U_0/(U_0 - 2U_2)$. If we consider the case with only two-sites, we obtain the spin-singlet (highest-spin) ground state if $U_2 > (<) 0$. In addition, it is known that at least in one-dimension, the ground state of this effective Hamiltonian is a dimerized state with a finite spin excitation gap if $U_2 > 0$, while the ground state is ferromagnetic state if $U_2 < 0$ [18]. The dimerized ground state with a positive U_2 suggests the polar state in the superfluid phase as we will see below.

To study the S-I transition, we use a mean-field approximation in Refs. [15] and [16]. We start from $t = 0$ case of Eq. 1, where the Hamiltonian is reduced to a diagonal matrix with respect to sites. Omitting the site index, the single-site Hamiltonian is

$$H_0 = -\mu\hat{n} + \frac{1}{2}U_0\hat{n}(\hat{n} - 1) + \frac{1}{2}U_2(\hat{\mathbf{S}}^2 - 2\hat{n}), \tag{2}$$

where $\hat{\mathbf{S}} = a_\alpha^\dagger \mathbf{F}_{\alpha\beta} a_\beta$ obeys a usual angular momentum commutation relation $[\hat{S}_i, \hat{S}_j] = i\epsilon_{ijk}\hat{S}_k$ and $\hat{n} = \sum_\alpha a_\alpha^\dagger a_\alpha$. $\hat{\mathbf{S}}^2$, $\hat{S}_z$, and $\hat{n}$ commute with each other. Therefore, the eigenstates of the above Hamiltonian are $|S, m; n\rangle (-S \le m \le S)$, where $\hat{\mathbf{S}}^2|S, m; n\rangle = S(S + 1)|S, m; n\rangle$, $\hat{S}_z|S, m; n\rangle = m|S, m; n\rangle$, and $\hat{n}|S, m; n\rangle = n|S, m; n\rangle$. The energy of the eigenstate is $E^{(0)}(S, n) = -\mu n + \frac{1}{2}U_0 n(n - 1) + \frac{1}{2}U_2[S(S + 1) - 2n]$. Since the orbital wave function is symmetric, the spin wave function has to be symmetric. As a result, $S = 0, 2, 4, ..., n$, when the number of atoms n is even and $S = 1, 3, 5, ..., n$, when n is odd [19]. The state with $m = S$ is $|S, S; n\rangle \propto (a_1^\dagger)^S (\Theta^\dagger)^{(n-S)/2}|vac\rangle$ [8], where $\Theta^\dagger \equiv {a_0^\dagger}^2 - 2{a_1}^\dagger {a_{-1}}^\dagger$ creates a spin-singlet pair. We obtain other states with lower magnetic quantum numbers by operating

$S^- = (S^+)^\dagger$ to $|S,S;n\rangle$, where $S^+ = S_x + iS_y = \sqrt{2}(a_1{}^\dagger a_0 + a_0{}^\dagger a_{-1})$. Since we assume an antiferromagnetic interaction, the ground state is $|0,0;n\rangle$ with $n/2$ singlet pairs if n is even, whereas the ground state is $|1,m;n\rangle (m = 0, \pm 1)$ if n is odd. Comparing $E_n^{(0)}$, $E_{n+1}^{(0)}$ and $E_{n+2}^{(0)}$, we obtain the relation between the number of the atoms per site in the ground state and the chemical potential (Fig.1). Note that if $U_0 < 2U_2$, the atom number per site is even all over the phase diagram.

Let us consider the case of finite t to study the superfluid transition. Here, we introduce the superfluid order parameter $\psi_\alpha = \langle a_{i\alpha}\rangle = \sqrt{n_0}\zeta_\alpha$, where n_0 is the superfluid density and ζ_α is a normalized spinor $\zeta_\alpha^*\zeta_\alpha = 1$. The hopping term is decoupled as $a_{i\alpha}^\dagger a_{j\alpha} \sim (\psi_\alpha a_{i\alpha}^\dagger + \psi_\alpha^* a_{j\alpha}) - \psi_\alpha^*\psi_\alpha$. As a result, the Hamiltonian is represented by a site-independent effective Hamiltonian multiplied by the total number of sites. The effective mean-field Hamiltonian [15, 16] is

$$\begin{aligned} H_{\mathrm{mf}} =& \quad H_0 + zt\sum_\alpha \psi_\alpha^*\psi_\alpha + V, \\ V =& \quad -zt\sum_\alpha (\psi_\alpha^* a_\alpha + \psi_\alpha a_\alpha^\dagger), \end{aligned} \tag{3}$$

where z is the number of the nearest-neighbor sites. V corresponds to the transfer between bosons localized on a particular site and the superfluid. We assume ψ_α and t are small and include V by a perturbation theory.

We first consider the case when the number of atoms in a site is even. Calculating the second-order correction, we obtain the ground state energy as

$$\begin{aligned} &\bar{E}_n(\psi) = \bar{E}^{(0)}(0,n) + A\left(n, \bar{U}_0, \bar{U}_2, \bar{\mu}\right)(\vec{\psi}^\dagger \cdot \vec{\psi}), \\ &A\left(n, \bar{U}_0, \bar{U}_2, \bar{\mu}\right) = \Bigg[1 + \frac{1}{3}\Big(\frac{n+3}{\bar{\mu} - \bar{U}_0 n} \\ &+ \frac{n}{-\bar{\mu} + \bar{U}_0(n-1) - 2\bar{U}_2}\Big)\Bigg], \end{aligned} \tag{4}$$

where $\bar{E} \equiv E/zt$, $\bar{\mu} \equiv \mu/zt$, $\bar{U}_F \equiv U_F/zt$ and $\vec{\psi} \equiv (\psi_1, \psi_0, \psi_{-1})$. Since the order parameter is determined to minimize the ground state energy, the ground state is the insulating (superfluid) phase with zero (finite) $\vec{\psi}$ if $A > (<) 0$. By the condition $A = 0$, we obtain the

upper (μ_+) and lower (μ_-) phase boundaries as

$$\begin{aligned}\bar{\mu}_{\pm} = \quad & -\bar{U}_2 + \frac{1}{2}[(2n-1)\bar{U}_0 - 1] \\ & \pm\frac{1}{6}\Big\{9\bar{U}_0^2 + 6\left(6\bar{U}_2 - 2n - 3\right)\bar{U}_0 \\ & +[36\bar{U}_2^2 - 12(2n+3)\bar{U}_2 + 9]\Big\}^{1/2}. \end{aligned} \tag{5}$$

By equating $\bar{\mu}_+$ and $\bar{\mu}_-$, we find the minimum of $\bar{U}_0$, denoting $\bar{U}_0^c$. The result is

$$\bar{U}_0^c = -\frac{1}{3}[6\bar{U}_2 - (2n+3)] + \frac{2}{3}\sqrt{n^2+3n}. \tag{6}$$

The results obtained by the second order perturbation with V cannot determine the symmetry of the superfluid order parameter. In order to determine this, we have to calculate the fourth-order perturbation energy $E^{(4)} = \sum_{n,p,q\neq i}\langle i|V|n\rangle\frac{\langle n|V|p\rangle}{E_i^{(0)}-E_n^{(0)}}\frac{\langle p|V|q\rangle}{E_i^{(0)}-E_p^{(0)}}\frac{\langle q|V|i\rangle}{E_i^{(0)}-E_q^{(0)}} - E^{(2)}\sum_n\frac{|\langle i|V|n\rangle|}{(E_i^{(0)}-E_n^{(0)})^2}$[20]. A long but straightforward calculation gives

$$\begin{aligned}\bar{E}_n^{(4)} = \quad & B\left(n,\bar{U}_0,\bar{U}_2,\bar{\mu}\right) n_0^2|\zeta_0^2 - 2\zeta_1\zeta_{-1}|^2 \\ & +C\left(n,\bar{U}_0,\bar{U}_2,\bar{\mu}\right)(\vec{\psi}^\dagger\cdot\vec{\psi})^2, \end{aligned} \tag{7}$$

with

$$
\begin{aligned}
B\left(n,\bar{U}_0,\bar{U}_2,\bar{\mu}\right) = \; & -\frac{1}{9}\left[\frac{n(n+1)}{\Delta\bar{E}^{(0)}(1,n-1)^2\Delta\bar{E}^{(0)}(0,n-2)}\right. \\
& \left.+\frac{(n+2)(n+3)}{\Delta\bar{E}^{(0)}(1,n+1)^2\Delta\bar{E}^{(0)}(0,n+2)}\right] \\
& +\frac{2}{45}\left[\frac{n(n-2)}{\Delta\bar{E}^{(0)}(1,n-1)^2\Delta\bar{E}^{(0)}(2,n-2)}\right. \\
& \left.+\frac{(n+3)(n+5)}{\Delta\bar{E}^{(0)}(1,n+1)^2\Delta\bar{E}^{(0)}(2,n+2)}\right] \\
& -\frac{n(n+3)}{15}\left[\frac{1}{\Delta\bar{E}^{(0)}(1,n+1)}\right. \\
& \left.+\frac{1}{\Delta\bar{E}^{(0)}(1,n-1)}\right]^2\frac{1}{\Delta\bar{E}^{(0)}(2,n)}, \\
C\left(n,\bar{U}_0,\bar{U}_2,\bar{\mu}\right) = \; & -\frac{2}{15}\left[\frac{n(n-2)}{\Delta\bar{E}^{(0)}(1,n-1)^2\Delta\bar{E}^{(0)}(2,n-2)}\right. \\
& \left.+\frac{(n+3)(n+5)}{\Delta\bar{E}^{(0)}(1,n+1)^2\Delta\bar{E}^{(0)}(2,n+2)}\right] \\
& +\frac{n(n+3)}{45}\left[\frac{1}{\Delta\bar{E}^{(0)}(1,n-1)}\right. \\
& \left.+\frac{1}{\Delta\bar{E}^{(0)}(1,n+1)}\right]^2\frac{1}{\Delta\bar{E}^{(0)}(2,n)} \\
& +\frac{1}{9}\left[\frac{n}{\Delta\bar{E}^{(0)}(1,n-1)}+\frac{n+3}{\Delta\bar{E}^{(0)}(1,n+1)}\right] \\
& \left[\frac{n}{\Delta\bar{E}^{(0)}(1,n-1)^2}+\frac{n+3}{\Delta\bar{E}^{(0)}(1,n+1)^2}\right],
\end{aligned} \tag{8}
$$

where $\Delta E^{(0)}(S,l) \equiv E^{(0)}(S,l) - E^{(0)}(0,n)$. The first term on the right-hand side of Eq. 7 lifts the degeneracy of the superfluid order parameters in spin space. Because $B\left(n,\bar{U}_0,\bar{U}_2,\bar{\mu}\right)$ is negative with even n, the superfluid phase is a polar (spin-0) state $\vec{\zeta} = (0,1,0)$ as in the spin-1 Bose condensation in a usual harmonic trap [12]. The fourth-order calculation is explained physically. The second intermediate states are $|0,0;n\pm 2\rangle$, $|2,m;n\pm 2\rangle$, and $|2,m;n\rangle$. The processes passing through $|0,0;n\pm 2\rangle$ ($|2,m;n\pm 2\rangle$) makes negative (positive) contributions to $B\left(n,\bar{U}_0,\bar{U}_2,\bar{\mu}\right)$ which favors (disfavors) the polar state. This is physically natural since $|0,0;n\pm 2\rangle$ ($|2,m;n\pm 2\rangle$) contains a spin-singlet (triplet) pair. Other processes passing through $|2,m;n\rangle$ make nontrivial negative contributions to $B\left(n,\bar{U}_0,\bar{U}_2,\bar{\mu}\right)$. Adding all these contributions, we obtain a negative $B\left(n,\bar{U}_0,\bar{U}_2,\bar{\mu}\right)$, therefore the superfluid is the polar state.

Now consider the case where the number of atoms per site is odd. Since the non-

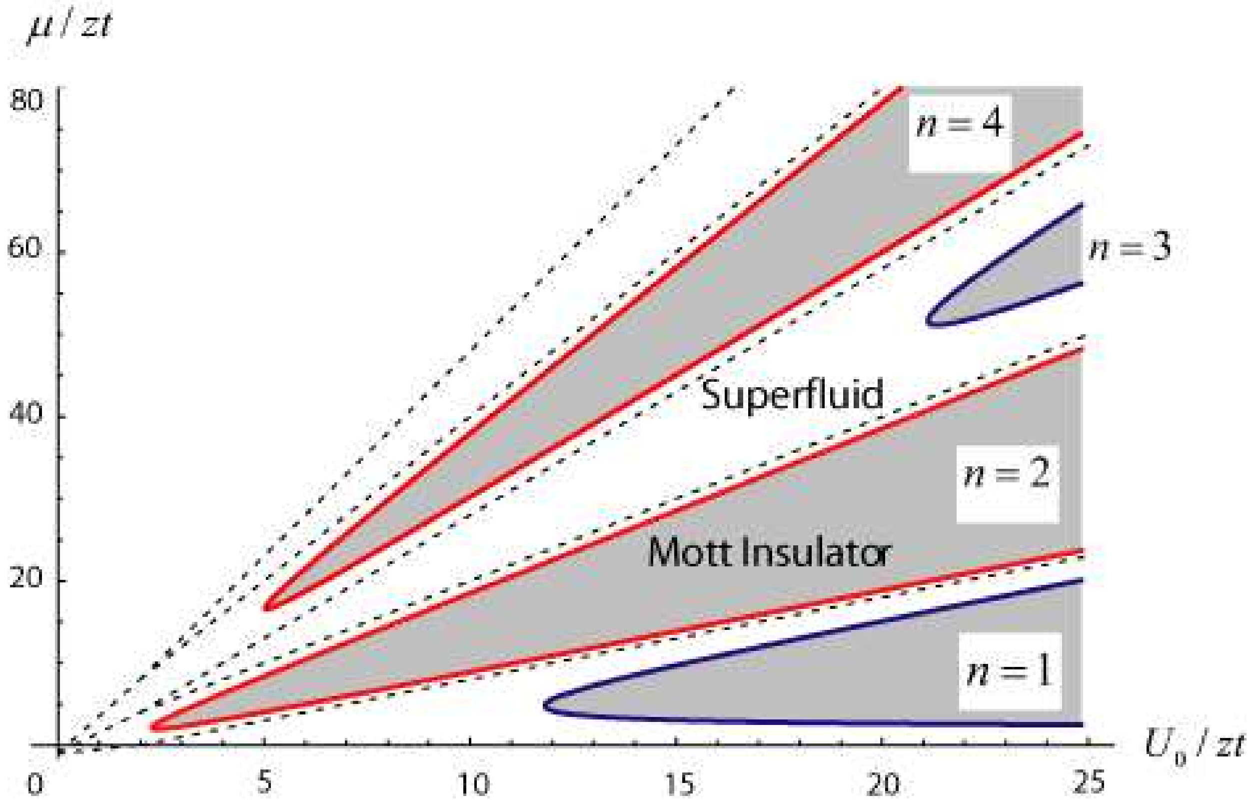

FIG. 1: Phase diagram of bose-Hubbard model with spin degrees of freedom when $U_2/zt = 1$. The dark region represents the Mott-insulating phase. The dashed lines indicate the phase boundaries at $t = 0$.

perturbative ground state has degenerated states with $m = 0$ and ± 1, we have to solve the secular equation $\Big| \langle 1, m; n | V \frac{1}{E^{(0)}(1,n) - H_0} V | 1, m'; n \rangle$
$- E_n^{(2)} \delta_{mm'} \Big| = 0$ to lift the degeneracy. The energy eigenvalues are obtained as

$$\begin{aligned} \bar{E}_n^{(2)} = \; & [-3(\beta+\delta) - (\alpha+\gamma) + 7(\beta+\delta)](\vec{\psi}^\dagger \cdot \vec{\psi}), \\ & \pm \Big\{ [(\alpha-\gamma) - 5(\beta-\delta)]^2 (\vec{\psi}^\dagger \cdot \vec{\psi})^2 \\ & +4(3\beta+\gamma-2\delta)(\alpha-2\beta+3\delta) n_0^2 |\zeta_0^2 - 2\zeta_1\zeta_{-1}|^2 \Big\}^{1/2}, \end{aligned} \tag{9}$$

where α,β,γ, and δ are given by $\alpha = \frac{n+2}{3} \frac{1}{\Delta \bar{E}^{(0)}(0,n-1)}$, $\beta = \frac{n-1}{15} \frac{1}{\Delta \bar{E}^{(0)}(2,n-1)}$, $\gamma = \frac{n+1}{3} \frac{1}{\Delta \bar{E}^{(0)}(0,n+1)}$, and $\delta = \frac{n+4}{15} \frac{1}{\Delta \bar{E}^{(0)}(2,n+1)}$ respectively and $\Delta E^{(0)}(S,l) \equiv E^{(0)}(S,l) - E^{(0)}(1,n)$. The ground state energy corresponds to the lower sign of Eq. 9. Since $(3\beta+\gamma-2\delta)(\alpha-2\beta+3\delta)$ is positive when n is odd, the ground state of superfluid phase is a polar state as the same as the case of even n.

Surprisingly, the Mott insulating phase with even n is strongly stabilized against the

superfluid phase comparing with odd-n case. This is intuitively understood as follows: in the case of even number of atoms per site, all atoms are able to form singlet pairs on each site, while in the case of odd number atoms, one atom remains to be made pairing. In the former case, the boson pairs are strongly localized on a site since the formation of singlet pairs prevent the bosons from hopping to the nearest-neighbor sites. Since the hopping is essential for the superfluid transition, the Mott insulating phase is stabilized in the former case. On the contrary, remaining one atom is free to hop to the nearest-neighbor sites more freely in the latter case, thus the superfluid transition occurs easily. In addition, Eq. 6 shows that U_0^c decreases linearly with U_2, which is consistent with the above consideration since the formation of singlet pairs is energetically more favorable when U_2 is larger.

This "even-odd conjecture" reminds us one-dimensional antiferromagnetic Heisenberg models (Haldane's conjecture) [21] and electronic ladder systems [22] such as Hubbard or $t-J$ ladders. Both systems show similar properties; the Haldane (ladder) systems have a spin excitation gap and an exponential decay of the spin correlation function with an integer spin (an even number of legs), while gapless and power-low decay with a half-integer spin (an odd number of legs). These properties are able to be essentially explained in terms of tightly bound spin singlets as the present study. However, we have applied this even-odd conjecture to the Bose systems or S-I transitions for the first time.

Finally we note that if we assume a ferromagnetic inter-atom interaction ($U_2 < 0$), there seems to be no strong even-odd dependence of the phase boundaries since the Mott insulator phase is the highest spin state and does not include singlet pairs. The detailed comparison between the ferromagnetic case and the present study remains as a future problem. Other possibilities such as fragmented condensates or two-particle pairings [23] should also be studied in this system.

To summarize, we have investigated the S-I transition of spin-1 bosons in an optical lattice. The zero-temperature phase diagram has been obtained by a mean-field theory. We have determined the order parameter of superfluid phase and showed that superfluid phase is a polar state. More interestingly, we have obtained a new kind of even-odd conjecture that the Mott insulating phase is strongly stabilized against the superfluid phase only when the number of atoms per site is even.

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